Finite temperature hole dynamics in the t–J model: exact results for high dimensions

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Abstract. – We discuss the dynamics of a single hole in the $t-J$ model at finite temperature, in the limit of large spatial dimensions. The problem is shown to yield a simple and physically transparent solution, that exemplifies the continuous thermal evolution of the underlying string picture from the $T = 0$ string-pinned limit through to the paramagnetic phase.

Following early pioneering work [1,2], and given added impetus by the discovery of high-T_c superconductivity, the study of single-particle excitations in magnetic insulators remains highly topical. At possibly its simplest, the dynamics of a single hole in an antiferromagnet (AF) is captured by the $t - J$ model [3], itself the strong coupling limit of the Hubbard model and a paradigm for the physics of strong, local electron correlations: hole motion, with nearest neighbour (NN) hopping amplitude t, occurs in a restricted subspace of no doubly occupied sites, and in a background of AF coupled spins with NN exchange couplings $J = 4t^2/U$. The string picture (see *e.g.* [4,5]), wherein the hole is pinned by the string of upturned spins its motion creates, has proven central in understanding the $t-J$ model at $T = 0$: since spins in the resultant string are flipped relative to the Néel configuration, resulting for $J > 0$ in energetically unfavourable exchange fields that generate a potential growing linearly with distance from its point of creation, the hole is thereby confined. And while string unwinding, and hence a finite hole mobility, is in general induced both by spin-flip interactions and Trugman loop motion [6], the underlying picture is robust even in $d = 2$ dimensions (see *e.g.*[5]).

The limit of large spatial dimensions, $d = \infty$, has also proven highly fruitful in study of the $t-J$ model [7-11]. Here the string picture has been shown to be exact, and the model solved at $T = 0$ [7,8]; the additional roles of disorder [8], and of second NN hopping [9], have also been investigated. Moreover, in addition to providing exact solutions, the d^∞ limit serves as a starting point for $1/d$ expansions, enabling a systematic approach to the finite-d case.

Given the success and utility of the large-d approach, we use it here to investigate another key element of hole dynamics in the t-J model: the role of temperature. That the spectrum of single-particle excitations, and hole conductivity, should change radically with T on the scale of the Néel temperature T_N, is easily understood; for while the two-sublattice A/B

structure characteristic of the Néel ordered AF phase persists for $0 < T < T_N$, the sublattice magnetization is not saturated: $m(T) < m(0) = 1/2$. In contrast to the $T = 0$ limit, therefore, *any* site has a non-zero probability $p_{\alpha\sigma}$ (where α=A or B distinguishes the sublattices) of being occupied by an electron of either spin type, $\sigma = +/-$ or $\uparrow/\downarrow$. In consequence, single-step hole motion may incur either an exchange energy penalty — if a spin hops to the 'wrong' sublattice, as occurs inevitably at $T = 0$ — or an energy *gain* if the converse occurs; and since spins in the string need not therefore be energetically penalized, a finite hole mobility results. Hole dynamics thus change character entirely on the scale of T_N itself, since in the paramagnetic phase for $T > T_N$, where $m(T) = 0$, the energy barrier to hole motion vanishes, and the hole propagates essentially as a free particle. In this Letter we show that an exact, yet rather simple and physically transparent, solution to the problem can be given; providing in addition a benchmark against which approximations, such as the NCA [10,11], can be judged.

The $t-J$ Hamiltonian $\hat{H} = \hat{H}_t + \hat{H}_J$ is given in standard notation by

$$\hat{H} = -t \sum_{i,j,\sigma} \tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} + \tfrac{1}{2} J \sum_{i,j} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \quad ; \tag{1}$$

the sums are over NN sites, and $\tilde{c}_{i\sigma}^\dagger = c_{i\sigma}^\dagger (1 - \hat{n}_{i-\sigma})$ embodies the constraint of no double occupancy by electrons. To ensure a well behaved limit for $d = \infty$, the hopping and exchange couplings are scaled as

$$t = t_*/\sqrt{Z} \ , \quad J = J_*/Z \tag{2}$$

with $Z \to \infty$ the coordination number ($Z = 2d$ for a hypercubic lattice). Spin-flip interactions are wholly suppressed for d^∞ (they contribute to $O(1/d)$), see *eg.*[7,8]; whence $\hat{H}_J \to \frac{1}{2} J \sum_{i,j} \hat{S}_i^z \hat{S}_j^z$, simple molecular field theory (MFT) for which becomes trivially exact for d^∞. To study hole dynamics we consider the thermally averaged, local one-hole Green function (retarded), given by

$$\overline{G}_{ii}(\omega) = \sum_s P(s) \langle i; s | (z - \hat{H}')^{-1} | i; s \rangle \quad ; \tag{3}$$

$|i; s\rangle$ denotes the hole on site i with configuration $s = \{\sigma_k\}$ for the remaining spins, with energy E_s under $\hat{H}_J$; $\hat{H}' = \hat{H} - E_s$ and $z = \omega + i0+$. $G_{ii}(\omega) = \langle i; s | (z - \hat{H}')^{-1} | i; s \rangle$ is the local Green function for the given configuration s, the probability $P(s)$ of generating which is given exactly for d^∞ by $P(s) = \prod_{k(\neq i)} p_k(\sigma_k)$ (with corrections $O(1/d)$), reflecting the statistical independence inherent in d^∞. Here $p_k(\sigma_k)$, such that $p_k(\sigma) = p_{\alpha\sigma}$ for site k belonging to the $\alpha = A$ or B sublattice (with $p_{A\sigma} = p_{B-\sigma}$), is given by

$$p_{\alpha\sigma} = \tfrac{1}{2} [1 + 2\lambda_\alpha \sigma m(T)] \tag{4}$$

with $\lambda_\alpha = +1(-1)$ for $\alpha = A(B)$; and the sublattice magnetization is given from simple MFT by

$$m(T) = \tfrac{1}{2} \tanh \left[\frac{2T_N}{T} m(T) \right] \tag{5}$$

with $T_N = \frac{1}{4} J_*$ ($k_B = 1$) the associated Néel temperature.

To obtain $G_{ii}(\omega)$ for an arbitrary configuration s, as now sketched, we first introduce a Feenberg self-energy $S_i(\omega)$ via

$$G_{ii}(\omega) = [z - S_i(\omega)]^{-1} \quad . \tag{6}$$

To obtain $S_i(\omega)$ one may proceed thus: (a) Separate the resolvent operator $\hat{G}=(z-\hat{H}')^{-1}$ as $\hat{G}=\hat{G}_0+\hat{G}_0\hat{H}_t\hat{G}$, where $\hat{G}_0=(z-\hat{H}'_J)^{-1}$ with $\hat{H}'_J=\hat{H}'-E_s$, such that $\langle j;s'|\hat{G}_0|i;s\rangle=\delta_{ij}\delta_{ss'}/z$; (b) take matrix elements of $\hat{G}$ between $\langle j;s'|$ and $|i;s\rangle$, obtaining thereby an 'equation of motion' for $G_{ji}(\omega)=\langle j;s'|\hat{G}|i;s\rangle$ which (c) may then be iterated perturbatively in t. This generates the Nagaoka path formalism [1,2], enabling systematic construction of $S_i(\omega)$ in unrenormalized form, *i.e.* as an explicit function of frequency ω. The Nagaoka path formalism is however a particular case of the Feenberg perturbation series (see *e.g.*[12]), the general power of which is to express $S_i(\omega)$ in *renormalized* form — *i.e.* as an explicit functional of the $\{G_{jj}\}$ — enabling from Eq.(6) a self-consistent solution for the $\{G_{jj}\}$.

The problem is particularly clear for the $Z\to\infty$ Bethe lattice, on which we focus explicitly (the hypercube can also be handled, the same physical ideas being involved but the algebra more complex). Here, $S_i(\omega)$ is given by

$$S_i = \sum_{j,s'}\langle i;s|\hat{H}_t|j;s'\rangle\langle j;s'|(z-\hat{H}')^{-1}|j;s'\rangle\langle j;s'|\hat{H}_t|i;s\rangle \quad , \tag{7}$$

where since hopping is solely NN, the spin configuration s', with energy $E_{s'}$ under $\hat{H}_J$, differs from s only by a *single* hole/electron transfer; and $\langle j;s'|\hat{H}_t|i;s\rangle\equiv -t$. From the energy change involved in transferring a σ_j-spin electron on site j in configuration s to an empty site i, it follows simply that $E_{s'}=E_s+\lambda_j\sigma_j\omega_p(T)$, reflecting either the energy cost ($\lambda_j\sigma_j=+1$) or gain ($\lambda_j\sigma_j=-1$) under single-step hole motion; here

$$\omega_p(T) = J_*m(T) \tag{8}$$

is the magnitude of the energy incurred in hole transfer which, involving necessarily sites on different sublattices, is equivalent to the exchange energy cost for an on-site spin-flip from $\sigma=+(-)$ to $-(+)$ on an $A(B)$ sublattice site. From this it follows straightforwardly that for $Z\to\infty$, $\langle j;s'|(z-\hat{H}')^{-1}|j;s'\rangle=G_{jj}(\omega-\lambda_j\sigma_j\omega_p(T))$, whence as sought Eq.(7) yields S_i as a functional of the $\{G_{jj}\}$:

$$S_i=t^2\sum_j G_{jj}(\omega-\lambda_j\sigma_j\omega_p(T)) \tag{9a}$$

(with sites j NN to i). The thermal average of S_i, denoted by $\overline{S}$ (and naturally independent of the sublattice index i), follows directly noting likewise that $\overline{G}_{ii}\equiv\overline{G}$ is independent of i:

$$\overline{S} = t_*^2\sum_\sigma p_{\alpha\sigma}\overline{G}(\omega-\lambda_\alpha\sigma\omega_p(T)) \tag{9b}$$

Finally, we recognize that $\overline{G}=\overline{[z-S_i]^{-1}}$ reduces simply to $\overline{G}=[z-\overline{S}]^{-1}$ for $Z\to\infty$ (the corrections being $O(Z^{-1})$). Hence the desired result

$$\overline{G}(\omega) = \left[z-t_*^2\left(p_{B\downarrow}\overline{G}(\omega-\omega_p(T))+p_{B\uparrow}\overline{G}(\omega+\omega_p(T))\right)\right]^{-1} \tag{10}$$

where $p_{B\sigma}(=p_{A-\sigma})$ and $\omega_p(T)$ are given from Eqs.(4,8) solely in terms of the sublattice magnetization $m(T)$, whose T and J_* dependence follows explicitly from the simple MFT equation, Eq.(5).

Eq.(10) is exact and, with Eqs.(4,5,8), closed. Further, although we have merely sketched the derivation here its physical content is quite clear, involving simply the thermal probability ($p_{B\sigma}$ factors) with which a NN site to the initially created hole is occupied by a σ-spin electron, together with the associated energy cost/gain (the $\omega\mp\omega_p(T)$ shifts) incurred in NN hole transfer. For $T=0$, where $m(T)=\frac{1}{2}$ and hence $p_{B\sigma}=\delta_{\sigma\downarrow}$ and $\omega_p(0)=\frac{1}{2}J_*$, Eq.(10) reduces

to $\overline{G}(\omega) = [z - t_*^2 \overline{G}(\omega - \frac{1}{2}J_*)]^{-1}$, the well known exact d^∞ result from the $T = 0$ string picture [8] (and for finite-d an approximation often used in practice [13]), yielding the familiar discrete spectrum characteristic of the confined/localized hole. In the paramagnetic phase by contrast, $T \geq T_N = \frac{1}{4}J_*$, where $m(T) = 0 = \omega_p(T)$ and $p_{\alpha\sigma} = \frac{1}{2}$ $\forall$ α, σ, Eq.(10) reduces to $\overline{G}(\omega) = [z - t_*^2 \overline{G}(\omega)]^{-1}$, producing the semielliptic spectrum of full width $4t_*$ characteristic of free hole motion in the d^∞ Bethe lattice.

As a typical example, Fig.1 shows for $J_*/t_* = 0.4$ the resultant hole spectrum $D(\omega) = -\pi^{-1} \text{Im } \overline{G}(\omega)$ at four different T's; the spectral sum rule $\int_{-\infty}^{\infty} d\omega D(\omega) = 1$ is always satisfied. From Eq.(10), the thermal evolution of $D(\omega)$ is controlled by that of the sublattice magnetization $m(T)$, Eq.(5). At the lowest T shown, $T = 0.3T_N$, $m(T)$ remains close to saturation: $m(T)/m(0) \simeq 0.997$. Hence $D(\omega)$ resembles closely its discrete $T = 0$ counterpart: the peak positions coincide, with only minor thermal broadening. Increasing T to $0.5T_N$ produces a modest reduction in $m(T)$ to $\sim 0.96m(0)$, but an appreciable effect upon $D(\omega)$, with increased broadening and the incipient formation of a background continuum. The latter, a precursor of free-hole dynamics, grows with increasing T; see Fig.1(c) for $T = 0.7T_N$ where $m(T) \simeq 0.83m(0)$. By $T = 0.9T_N$ where $m(T) \simeq 0.53m(0)$, the semiellipse characteristic of free hole motion is clearly emerging, Fig.1(d), showing also that the 'shortest strings' — those to the low-ω side of $D(\omega)$ — are the last to be thermally eroded. Finally, in the paramagnet for $T > T_N = \frac{1}{4}J_*$, the resultant semielliptic $D(\omega)$ is independent of T for obvious physical reasons.

Fig.1 shows clearly that while the effective spectral width is on the scale of the hopping t_*, the essential character of the spectrum evolves on the typically much smaller scale of $T_N = \frac{1}{4}J_*$ ($= 0.1t_*$ in Fig.1). Qualitatively similar behaviour occurs on varying J_*/t_*; the rule of thumb being that for any fixed T/T_N (and hence constant $m(T)$ and $p_{\alpha\sigma}$, see Eqs.(4,5)), increasing J_* amplifies the hole transfer shifts in Eq.(10) (since $\omega_p(T) = J_*m(T)$), thus producing a somewhat 'colder' spectrum.

The behaviour described above is reflected also in the hole conductivity $\sigma(\omega; T)$, itself of $O(1/d)$ in high dimensions but with $\sigma(\omega; T)/t^2$ (or equivalently $\text{Tr}\sigma_{\lambda\lambda}(\omega; T)$) of order unity and a much studied quantity [7,8]. Due to the absence of vertex corrections for d^∞, the (real) dynamical conductivity $\sigma(\omega; T)$ is expressible in terms of the hole spectrum $D(\omega)$; and an exact expression for it may be deduced along the lines sketched above for $D(\omega)$. We quote only the result (which is independent of lattice type), namely

$$\sigma(\omega; T) \propto \frac{(1 - e^{-\beta\omega})}{\omega} \frac{\int_{-\infty}^{\infty} d\omega_1 e^{-\beta\omega_1} D(\omega_1) \left[p_{B\downarrow} D\left(\omega_1 + \omega - \omega_p(T)\right) + p_{B\uparrow} D\left(\omega_1 + \omega + \omega_p(T)\right) \right]}{\int_{-\infty}^{\infty} d\omega_1 e^{-\beta\omega_1} D(\omega_1)} \quad (11)$$

where $\beta = 1/T$ and extraneous constants have been dropped for clarity. Temperature enters Eq.(11) in two ways: via (a) explicit Boltzmann factors and (b) the T-dependence of $D(\omega)$, $p_{B\sigma}$ and $\omega_p(T)$. In previous work [8] the latter have been neglected entirely and replaced by their $T = 0$ counterparts with $p_{B\sigma} = \delta_{\sigma\downarrow}$ and $\omega(0) = \frac{1}{2}J_*$, whereupon Eq.(11) reduces to the result of [8]. This amounts to retaining only the $T = 0$ Néel spin configuration in calculating $\sigma(\omega; T)$, but is not a physically realistic approximation: since $D(\omega)$ for $T = 0$ is discrete, the dynamical conductivity consists of a series of δ-functions whose weight alone depends on T [8], and the dc conductivity $\sigma_0(T) = \sigma(\omega = 0; T)$ vanishes for all T. While the introduction of disorder [8] broadens the δ-peaks and leads to non-trivial behaviour, the absence of a proper T-dependence limits somewhat the utility of this approximation.

Eq.(11) by contrast is exact at finite-T. To illustrate it, Fig.2 gives the resultant dc conductivity $\sigma_0(T)/\sigma_0(T_N)$ *vs.* T/T_N for $J_*/t_* = 0.4$. As expected it is $T_N = \frac{1}{4}J_*$, and not the hopping t_* ($= 10T_N$ in Fig.2), that sets the scale for the T-dependence of the conductivity in the AF phase. $\sigma_0(T)$ is non-zero for any $T > 0$, reflecting the fact that

true hole confinement/localization is exclusively a $T = 0$ phenomenon, as embodied also in the corresponding loss of the discrete $T = 0$ hole spectrum at finite T (Fig.1); the progressive increase of $\sigma_0(T)$ with T in the AF phase likewise reflects the enhanced thermal broadening of $D(\omega)$. At $T = T_N$ the conductivity acquires a sharp cusp, across which $d\sigma_0(T)/dT$ changes sign. In the paramagnetic phase, $p_{\alpha\sigma} = \frac{1}{2}$, $\omega_p = 0$ and (see Eq.(10)) $D(\omega)$ is independent both of T and J_*: Eq.(11) for $\sigma(\omega; T)$ thus reduces in practice to its well known $J_* = 0$ limit [7,8]. For $T > T_N$ the T-dependence of $\sigma_0(T)$ is thus controlled by the *sole* remaining scale, t_*, diminishing monotonically with increasing T and approaching $\sigma_0(T) \sim 1/T$ behaviour for $T/t_* \gtrsim 1 - 2$ (which asymptote is evident from the $\beta = 1/T$ prefactor in Eq.(11) for $\omega = 0$).

In summary we have shown that in the large dimensional limit, the finite temperature dynamics of a single hole in an AF, as described by the $t - J$ model, admits to a simple closed solution that captures in a physically transparent fashion the continuous thermal evolution of the underlying string picture, from the $T = 0$ string-pinned limit to the paramagnetic phase $T > T_N$ where there is no exchange energy barrier to hole propagation. Although for clarity we have focussed explicitly on the Bethe lattice, the analysis is readily extended both to lattices with non-retraceable paths and, relatedly, to the case of a second NN hopping, which even for a Bethe lattice involves non-retraceable loop paths and likewise admits to a closed solution for all T [14]. The additional effects of disorder, as hitherto considered for $T = 0$ [8], are also easily encompassed; this, together with an elaboration of the present work, will be described in a subsequent paper.

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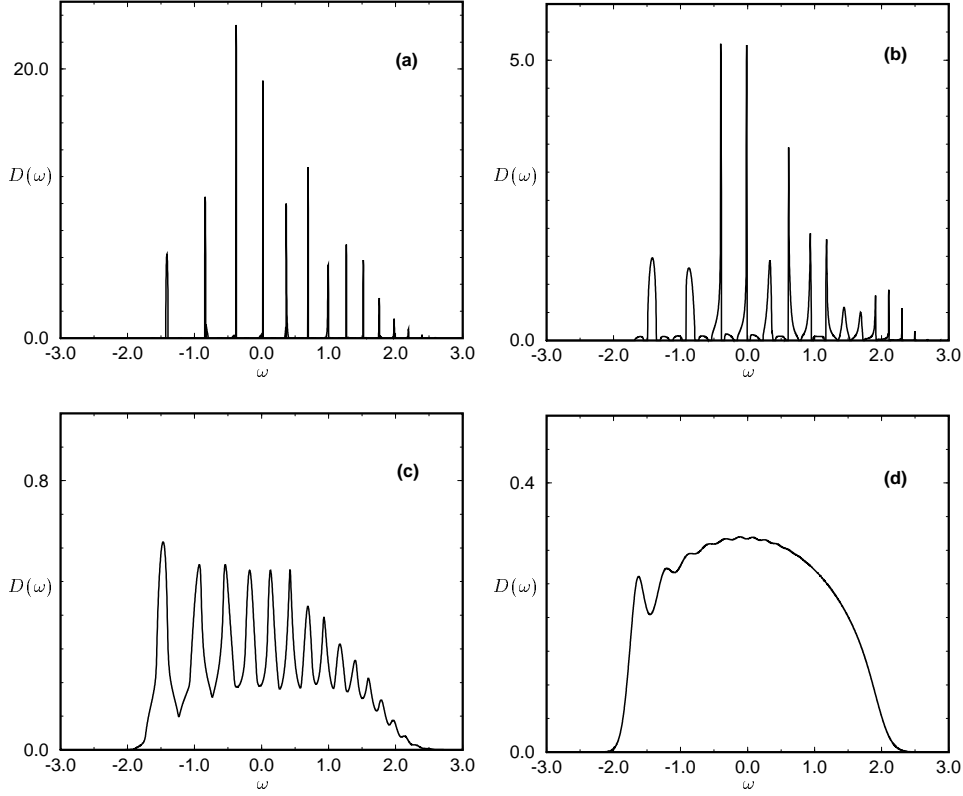[14] DICKENS N.L. and LOGAN D.E, *in preparation*.

Fig. 1. – Hole spectrum $D(\omega)$ *vs.* ω/t_* for $J_*/t_* = 0.4$ and $T/T_N = 0.3$ (a), 0.5 (b), 0.7 (c) and 0.9 (d); the Néel temperature $T_N = \frac{1}{4}J_*$.
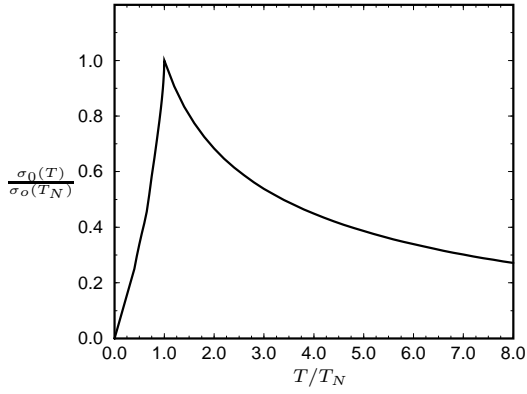

Fig. 2. – Static conductivity $\sigma_0(T)/\sigma_0(T_N)$ *vs.* T/T_N for $J_*/t_* = 0.4$. Note that $T_N = t_*/10$.